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Quality Assurance of NUFT Code for Underground Test Area (UGTA) Activities

S. F. Carle, Y. Hao, A. Tompson

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Contents

1 Introduction

The Underground Test Area (UGTA) Quality Assurance Plan (QAP), Revision 1, dated October 23, 2012 (USDOE, 2012) includes software quality assurance (QA) provisions applicable to groundwater flow/contaminant plume modeling codes used in UGTA activities. The Nonisothermal Unsaturated Flow and Transport (NUFT) numerical modeling code has been used in UGTA activities and is projected to be used in future UGTA activities. NUFT modeling activities for UGTA span a variety of simulation capabilities and processes including non-isothermal flow, variably saturated flow, gas and liquid phase flow, multi-component transport, and dual continuum (matrix and fracture) meshes (Maxwell et al., 2000; Pawloski et al., 2001; Carle et al. 2003, 2006a, 2006b, 2008). This report focuses on protection and justification of QA of NUFT following the UGTA QAP for computer software. Following a brief description and history of the NUFT code, this report addresses procedures for demonstrating compliance of NUFT within the UGTA QAP, specifically with respect to QA specifications for computer software and codes. This includes:

- Version Control
- Selection
- Development
- Verification
- Installation Testing
- Example Installation Test Procedure
- Code Review
- Configuration Control

2 NUFT Code

The Nonisothermal Unsaturated Flow and Transport (NUFT) code is a multipurpose numerical modeling software package designed for simulation of fluid flow and species mass transport processes in porous and fractured subsurface formations. NUFT includes unsaturated, multi-phase, non-isothermal, multi-component transport, and chemistry process modeling capabilities. NUFT can be used with both structured and unstructured meshes.

The NUFT source code was originally developed by John Nitao at Lawrence Livermore National Laboratory (LLNL). Yue Hao of LLNL currently provides support for NUFT source code and installation for a variety of LLNL programs, including the Underground Test Area Activity (UGTA). The currently-supported NUFT code includes five distinct modules with names that reflect their individual process capabilities:

- Unsaturated non-isothermal multi-phase flow and multi-component transport (USNT)
- Unconfined and confined aquifer and saturated flow (UCSAT)
- Unsaturated 1-phase flow (US1P)
- Unsaturated 1-component transport (US1C)
- Geochemical multiphase transport (TRANS)

The main documentation for NUFT is provided by a user manual (Nitao, 2000a) and a reference manual (Nitao, 2000b). Nitao (2004, 2005) and Lee (2000) provide more detailed documentation of the US1P and US1C modules and thermal input parameters. Nitao (2001) provides example applications and validation cases for NUFT.

USNT is the main or "unabridged" module for simulation of nonisothermal, multiphase subsurface flow and transport processes in NUFT. The process simulation capabilities of USNT were originally designed for use in the Yucca Mountain Project (YMP).

The UCSAT, US1P, and US1C modules are not separate codes from USNT, but, rather, simplified subsets of USNT with fewer process capabilities and input requirements to enable more efficient calculations in less complex process simulations. QA validation and verification testing of USNT effectively covers QA for UCSAT, US1P, and US1C. The NUFT executable for the USNT, UCSAT, US1P, and US1C modules has been publically available since 2007 through the LLNL Industrial Partnerships Office (https://ipo.llnl.gov) with a fee and end-user license. Public availability of NUFT provides an additional level of QA software verification that is achieved through multiple users and broader historical use.

The TRANS module is an independent body of code designed more recently for addressing geochemical reactive transport processes in porous media (Hao et al., 2012). It is part of the "NUFT-C" package (NUFT v4.0, see below) used internally at LLNL and is not currently available publically. The TRANS module to date has not been covered by the YMP or any other QA program. Because of its functional independence, the TRANS module does not affect QA of the USNT, UCSAT, US1P, and US1C modules.

3 Version Control

NUFT Version 4.0 (v4.0) is the current version of NUFT. Since 2005, NUFT v4.0 has been the NUFT version used for UGTA modeling activities as well as the supported version of NUFT at LLNL. Earlier versions of NUFT (v3.0 and earlier) received extensive QA under broad programmatic support of the Yucca Mountain Project (YMP). NUFT v4.0 was qualified for YMP use in 2007 (Section 2.3.3). Importantly, the thermohydrologic functionalities of NUFT v4.0 used for LLNL's UGTA modeling activities are effectively the same as those in NUFT v3.0 except for updated data tables (i.e., steam tables) to expand the range of pressure and temperature conditions that can be accommodated by NUFT. The main difference between NUFT v4.0 and NUFT v3.0 is the inclusion of the reactive transport (TRANS) module described above. QA activities applied to NUFT v3.0 and earlier are directly relevant to QA of NUFT v4.0 functionalities, modules, and code used in UGTA modeling activities except for the TRANS module.

4 Selection

Selection of NUFT for use in UGTA originated from similar functionality needs as for YMP. There are a limited number of codes with the functionality available to model hydrologic source term (HST) and other flow and transport processes needed for LLNL's UGTA modeling activities. In particular, only a few codes offer three-dimensional and multi-continuum modeling capabilities and address processes of multi-phase (or unsaturated) flow, one- or multi-component transport, and non-isothermal conditions. Codes historically developed for the Yucca Mountain Project (YMP) are the only publically available, non-commercial institutional codes with process capabilities needed for solving coupled mass and heat transport problems in geologic media as needed for UGTA. These codes include NUFT (Nitao, 2000a,b), TOUGH2 (Preuss, 2004), and FEHM (Zyvoloski, 2007).

There are several reasons NUFT was selected by LLNL for UGTA modeling activities:

- Functionality
- Flexibility
- Historical quality assurance under YMP
- Configuration Control
- History of Use
- Local Support

Further details on code selection are given below.

4.1 Functionality

Table 1 lists the functionality requirements satisfied by NUFT that meet longstanding specifications identified under YMP (Shaffer, 1999, 2000b).

Table 1. Functionality requirements of the NUFT software for YMP applications (Shaffer, 1999, 2000b).

Flow Processes	Pressure-driven gas flow Pressure-driven liquid flow Gravity effects Capillary effects Viscous forces
Flow Media	Porous Fractured Fractured/Porous
Constitutive Relations	Vapor pressure lowering Van Genuchten characteristic curve Temperature dependent capillary pressure
Fluid Phases	Single phase liquid flow Single phase gas flow Multi-phase flow Multi-component flow and transport Saturated flow Unsaturated flow
Phase Change/Diffusion	Phase change Phase (dis)appearance Binary diffusion in gas
Heat Transport	Conduction Convection Coupled fluid and heat flow Radiant heat transfer Isothermal Nonisothermal
Dimensionality	1-D, 2-D, 3-D
Sub-Models	Equivalent continuum model Dual permeability model (DKM) Active Fractures
Other	Automatic time stepping Nested meshes Evaporative flux Restart capability

The most recent YMP QA Requirements Document for NUFT v4.0 specifies code functionality requirements (FR), all of which are entirely transferable to the range in scope of UGTA modeling activities:

FR-1: *The software shall calculate flow processes including pressure-driven gas flow, pressure-driven liquid flow, gravity effects, capillary effects, and viscous force effects on flows.*

FR-2: *The software shall simulate flow processes in fractured porous media.*

FR-3: *The software shall provide constitutive relationships for vapor-pressure lowering, van Genuchten characteristic curves, and temperature-dependent capillary pressure.*

FR-4: *The software shall simulate single-phase liquid flow (saturated flow), single-phase gas flow, multiphase flow (unsaturated flow), and multi-component flow and transport.*

FR-5: *The software shall simulate phase changes, phase (disappearance, and binary diffusion in the gas phase.*

FR-6: *The software shall simulate heat transport in nonisothermal systems by convection, conduction, coupled fluid and heat flow, radiant heat transfer. Note that heat transport by thermal radiation shall only be simulated in the serial processing mode of the code.*

FR-7: *The software shall solve 1-, 2- and 3-dimensional flow and transport problems.*

FR-8: *The software shall provide equivalent continuum model (ECM) option, dual porosity/dual permeability model (also known as DKM) option, and active fracture model option.*

FR-9: *The software shall provide an anisotropic-thermal-conductivity option.*

FR10: *The software shall provide an automatic-time-stepping option.*

FR11*:* *The software shall provide a multilevel-nested-mesh option in serial processing mode.*

FR12*:* *The software shall provide evaporation/condensation-flux-output option.*

FR13: *The software shall provide a property-value-modification option for thermal conductivity and tortuosity.*

FR14*:* *The software shall provide an option to read an external-mesh file.*

FR15: *The software shall provide a restart capability.*

For LLNL's UGTA modeling activities, the most important functionality of NUFT is that it properly conserves fluid mass and momentum, species mass, and thermal energy under the governing equations of the mathematical model. Confidence in these functionalities is further assured when the flow, mass and heat transport parameters of a NUFT code application are within ranges utilized by NUFT validation studies (CRWMS M&O, 2007c).

4.2 Flexibility

"Flexibility" in the code refers to multipurpose capabilities for addressing physical and chemical processes and generating discretized numerical meshes. As introduced earlier, NUFT v3.0 and v4.0 include five "modules" of code with varying degrees of flow and transport process complexity:

- UCSAT – for modeling fully saturated single-phase flow under confined or unconfined conditions
- US1P – for modeling variably saturated single-phase flow using the Richards' Equation (Bear, 1972)
- US1C – for modeling transport of a single dissolved species (component) under variably saturated, liquid phase flow (Bear and Bachmat, 1991) using the same flow field and numerical conceptualization as in US1P
- USNT – for modeling multi-phase, multi-component, non-isothermal flow and transport
- TRANS – for geochemical multiphase reactive transport

The different modules enable faster and more efficient model implementation through simplification of input/output appropriate to process complexity. Over the course of LLNL's UGTA modeling activities since the late 1990s, all NUFT flow and transport process modules have been used. The flexibility and efficiency of having these five modules within the same flow and transport software package (versus having five separate software packages, for example) enables efficiencies in investigation of complex processes, integration of modeling results, and QA. For example:

- Single-phase flow in unsaturated conditions can be modeled independently of single-component transport using the US1P and US1C modules in tandem. This enables efficient staging of multiple radionuclide transport cases for the same flow case or visa-versa.
- Isothermal flow cases can be run with USNT and later extended to non-isothermal cases, if necessary. This enables a gradational increase of flow simulation complexity when considering thermal effects.
- Single-phase flow and single-component transport cases can be extended to multi-phase and multi-component cases using the same mesh with straightforward extension of component properties and initial and boundary conditions. This

enables gradational increase of flow simulation complexity when considering gas phase and multi-component flow and transport.

- The multipurpose capabilities eliminate need to transfer model input/output between multiple software packages. This eliminates need to translate file formats, model parameters, and units and, therefore, simplifies QA for transfer and transcription of data.

With respect to numerical mesh flexibility, NUFT provides several options which have been used or may have future usefulness for UGTA:

- Regularly spaced Cartesian meshes (internal mesh)
- Variably spaced Cartesian meshes (internal mesh)
- Nested Cartesian meshes (internal mesh)
- Multi-continuum meshes (internal mesh)
- Unstructured or irregular meshes (external mesh)

4.3 Historical Quality Assurance for the Yucca Mountain Project (YMP)

NUFT v2.0 and v3.0 underwent thorough quality assurance (QA) software verification and validation activities under broad YMP programmatic support (e.g., Lee et al., 1993; Shaffer and Fernandez, 1998; Shaffer, 2000a,b,c,d; Campbell, 2000; Nitao, 2001; CRWMS M&O, 2002). QA for NUFT v4.0 was continued under YMP (CRWMS M&O, 2007a) with independent validation and verification (CRWMS M&O, 2007b) and applications validation to later YMP multi-scale thermohydrologic modeling activities (CRWMS M&O, 2007c, 2008).

4.4 Configuration Control

Availability of configuration control support makes NUFT advantageous for use at LLNL compared to other codes of similar functionality. Under the YMP QA procedure for software configuration management (CWRMS M&O, 1999c), LLNL developed a software configuration management system (CWRMS M&O, 1998b; Campbell et al., 1999; Levitan and Lewis, 2000; Shaffer, 2000a). Configuration control for NUFT v4.0 was extended at LLNL as part of YMP QA assurance (CRWMS M&O, 2007a,c). LLNL currently supports control of NUFT software configuration for NUFT v4.0 on LLNL's institutional computer systems.

4.5 History of Use

NUFT has a long history of use in LLNL's UGTA HST modeling activities (Pawloski et al., 2001; Carle et al., 2003, 2006a, 2006b, 2008). Recently, NUFT has been used by Desert Research Institute's T-tunnel sub-CAU modeling (Navarro-INTERA, 2013). NUFT has also been used in numerous applications to nuclear waste repository siting and design (e.g., Buscheck et al., 2003; Glascoe et al., 2003; CWRMS M&O, 2007c), modeling groundwater systems (GMS, 2000), contaminant remediation (e.g., Newmark et al., 1998; Nitao, et al. 2000; Carrigan and Nitao, 2000; Sun, et al., 2000), radionuclide migration (Tompson et al., 2006), underground nuclear test detection (Carrigan et al., 1996; Vincent et al., 2011), geothermal energy (e.g., Tompson et al., 2013), and CO_2 geological sequestration (e.g., Johnson et al., 2004; Carroll et al., 2009; Morris et al., 2011; Lu et al., 2012; Sun et al., 2012; Hao et al., 2013). NUFT's availability to academic and commercial users broadens software verification through an outside user base.

4.6 Localized Support

As a code developed by and widely used in LLNL programs, localized support for NUFT is endemically available to LLNL's use of NUFT for UGTA activities. The broad LLNL user base and collaborative atmosphere among NUFT users at LLNL fosters efficient development and execution of UGTA modeling activities.

5 Development

NUFT code development is extensively documented. The code purpose, requirements, and activity lead consultations for development of NUFT v3.0 were documented in a software activity plan (Shaffer, 2000a). User and reference manuals (Nitao 2000 a,b) and supporting documents (e.g. Lee, 2000; Nitao, 2000c, Shaffer, 2000b) specify input and output requirements, assumptions, limitations on applications, operating systems, installation and execution instructions, and description of equations, algorithms, and numerical solution techniques. Nitao (2004, 2005) provide specifics on use of the US1P and US1P modules of NUFT. The NUFT installation test output file records the version date, operating system, and compilers for the installed NUFT version (Section 2.6). Further development details are provided in CWRMS M&O (2007c) as well as many of the references listed in Section 10.

6 Verification

Code verification for NUFT involves checking model output behavior for correctness with respect to known output or previous model results. Code verification of NUFT is accomplished in three ways:

- Historical use, which by nature includes peer review,
- Formalized benchmark, validation, or verification testing using test cases, and
- Application-oriented validation tests.

NUFT has a long history of use in thermohydrologic modeling beginning in the early 1990s in application to YMP (e.g., Buscheck and Nitao, 1992, 1993) including formalized verification testing (Lee et al., 1993). As of the early 2000s, a comprehensive series of validation test cases were developed in YMP for verification of the thermohydrologic modeling capabilities of NUFT v3.0 including:

- Eighteen benchmark tests examining accuracy of key functionalities,
- Six sample problems examining capability to simulate thermohydrologic phenomenon, and
- Seven verification tests of NUFT thermohydrologic process modeling capabilities.

Campbell (2000) and Shaffer (2000c, 2000d) document a formalized validation testing procedure for NUFT v3.0. Additional details on code verification requirements and testing for NUFT v3.0 can be found in Bechtel (2001) and CRWMS M&O (1998a, 1999a, 1999b).

The validation tests using NUFT v3.0 have been used for verification of the thermohydrologic modules of NUFT v4.0 (CWRMS M&O, 2007a). In 2007, NUFT v4.0 was qualified for YMP use on the SUN O.S. 5.8, AIX5.2 PSSP3.5, AIX5.3 CSM1.5, and CHAOS 3.1 computer system platforms (CWRMS M&O, 2007b).

Nitao et al. (2001) overviews several applied validation test cases using NUFT. Rigorous validation tests for YMP applications have been conducted to evaluate thermohydrologic response model results for NUFT v3.0 (CRWMS M&O, 2000a,b; Buscheck et al., 2002, 2003) and NUFT v4.0 (CRWMS M&O, 2005, 2007c). These validation tests verify NUFT output behavior with respect to (1) adequacy and accuracy of model output, (2) influence of parametric uncertainty, and (3) variability in geologic and hydrologic conditions. These YMP validation tests have direct relevance to UGTA QA for uncertainty analysis in that they were designed for evaluation and prediction over a wide range of thermohydrologic conditions as needed for UGTA HST modeling activities.

7 Installation Testing

NUFT was developed with a formalized installation test plan (Levatin and Lewis, 2000). The installation test plan includes specifications for pre-installation, installation, and an installation test. The installation test involves execution of NUFT with a test input file. The installation test produces an output file that is compared to a pre-existing installation test file to determine if the installation test is successful.

Under YMP software configuration management (SCM) responsibilities, installation testing was conducted when operation and hardware system configurations change (Campbell et al., 1999). The YMP SCM system stores verification documentation for installation testing including test inputs, test outputs, and certification documents. The NUFT installation tests developed for YMP are suitable for UGTA QA because computer systems and code applications are similar.

The installation test problem for the serial version of NUFT involves the following three files (in addition to a compiled version of NUFT):

- "`run_installation_test_ser`" — a job control script file to launch NUFT to run the test problem
- "`installation_test_ser.in`" — the input for the test problem
- "`installation_test_ser_exp.ex`" — the expected output to which results should be compared

The installation test output file "`installation_test_ser.ex`" includes the names of the operating system and compilers as required in UGTA QAP for software development (Section 2.1).

Current instructions for executing a NUFT installation test for serial processing, as used in LLNL's UGTA modeling activities, are listed below. The steps to performing the installation verification test for serial processing mode include:

- Locate the job control script file "`run_installation_test_ser`" in the directory.

- Edit "`run_installation_test_ser`" using any ASCII text editor such as emacs or vi so that "`<installation-test-dir>`" in the file is replaced by the full path of the current directory, and "`<nuft-dir>`" is replaced by the full path of the directory in which NUFT4.0 resides.

- Run the installation test by typing:

  ```
  csh run_installation_test_ser
  ```

- No error messages should be reported during the test run. A NUFT time history output file "`installation_test_ser.ex`" and a NUFT log file "`installation_test_ser.out`" should be generated after the test run. The expected time history output file "`installation_test_ser_exp.ex`" is also provided in the directory. The test results in "`installation_test_ser.ex`" should be the same as those in the expected time history output file.

An example installation test procedure is shown below in Section 2.6.1.

8 Example Installation Test Procedure

The installation test procedure shown below was implemented on the LLNL AZTEC computing cluster in May 2014:

1. The job control script was located:

```
[carle@aztec3 installation-test]$ ls -l *test_ser
-rwx------ 1 carle carle 203 Jan 27 11:43 run_installation_test_ser
```

2. The file "`run_installation_test_ser`" was edited and replaced by the full path of the directory in which NUFT resides:

```
#!/usr/bin/csh
# cd <installation-test-dir>
cd /g/g12/carle/nuft_QA/installation-test
# setenv NUFTPATH  <nuft-dir>
setenv NUFTPATH /g/g12/carle/nuft_05_ilx/src
$NUFTPATH/nuft installation_test_ser.in
```

3. The command "`csh run_installation_test_ser`" was typed at the command line prompt:

```
[carle@aztec3 installation-test]$ csh run_installation_test_ser
Copyright (c) 1994-2000. The Regents of the University of California.
All rights reserved.
NUFT version: cvs-11-17-04 (LINUX-GCC)
 >        "loading from directory: /g/g12/carle/nuft_05_ilx/src/"
 >        "loading /g/g12/carle/nuft_05_ilx/src/lsp/init.lsp"
reading input data file installation_test_ser.in
reading input data file /g/g12/carle/nuft_05_ilx/src/pkg/vtough.pkg
 > initializing model: usnt

note: init. values for some elements were overridden by values set in
boundary conditions, given in output file
*usnt(0) t 0.00e+00 ndt 1.0e+02 nr 0 lin 0
       max change P: 8.8e+04 dP: -3.1e+03 -- tsw35.f#1:1:2
*usnt(1) t 1.00e+02 dt 1.0e+02 ndt 1.9e+02 nr 2 lin 1
       max change P: 8.9e+04 dP: -9.4e+02 -- tsw35.f#1:1:4
*usnt(2) t 2.89e+02 dt 1.9e+02 ndt 4.0e+02 nr 2 lin 1
       max change P: 8.9e+04 dP: -5.4e+02 -- tsw35.f#1:1:11
*usnt(3) t 6.90e+02 dt 4.0e+02 ndt 8.7e+02 nr 2 lin 1
       max change P: 8.9e+04 dP: -2.6e+02 -- tsw35.f#1:1:16
*usnt(4) t 1.56e+03 dt 8.7e+02 ndt 1.9e+03 nr 2 lin 1
       max change P: 9e+04 dP: -3.2e+02 -- tsw35.m#1:1:2
*usnt(5) t 3.50e+03 dt 1.9e+03 ndt 4.3e+03 nr 2 lin 1
       max change P: 9e+04 dP: -5.8e+02 -- tsw35.m#1:1:2
```

```
*usnt(6) t 7.77e+03 dt 4.3e+03 ndt 9.3e+03 nr 2 lin 1
       max change P: 8.9e+04 dP: -8.9e+02 -- tsw35.m#1:1:2
*usnt(7) t 1.70e+04 dt 9.3e+03 ndt 2.0e+04 nr 2 lin 1
       max change P: 8.8e+04 dP: -9.9e+02 -- tsw35.m#1:1:2
*usnt(8) t 3.68e+04 dt 2.0e+04 ndt 4.2e+04 nr 2 lin 1
       max change P: 8.7e+04 dP: -7.3e+02 -- tsw35.m#1:1:2
*usnt(9) t 7.87e+04 dt 4.2e+04 ndt 9.0e+04 nr 2 lin 1
       max change P: 8.7e+04 dP: -3.3e+02 -- tsw35.m#1:1:4
*usnt(10) t 1.69e+05 dt 9.0e+04 ndt 2.0e+05 nr 2 lin 1
       max change S.gas: 0.98 dS.gas: -0.0047 -- tsw35.f#1:1:2
*usnt(11) t 3.67e+05 dt 2.0e+05 ndt 4.4e+05 nr 2 lin 1
       max change S.liquid: 0.029 dS.liquid: 0.0099 -- tsw35.f#1:1:2
*usnt(12) t 8.07e+05 dt 4.4e+05 ndt 9.6e+05 nr 2 lin 1
       max change S.gas: 0.97 dS.gas: -0.015 -- tsw35.f#1:1:3
*usnt(13) t 1.76e+06 dt 9.6e+05 ndt 2.0e+06 nr 3 lin 1
       max change S.liquid: 0.041 dS.liquid: 0.029 -- tsw35.f#1:1:4
*usnt(14) t 3.80e+06 dt 2.0e+06 ndt 4.2e+06 nr 7 lin 1
 ==> usnt, hit max. NR iterations, cut back to dt = 2.08e+06
       max change S.liquid: 0.04 dS.liquid: 0.03 -- tsw35.f#1:1:10
*usnt(15) t 5.88e+06 dt 2.1e+06 ndt 2.1e+06 nr 6 lin 1
       max change S.liquid: 0.041 dS.liquid: 0.031 -- tsw35.f#1:1:15
*usnt(16) t 7.96e+06 dt 2.1e+06 ndt 4.2e+06 nr 6 lin 1
 ==> usnt, hit max. NR iterations, cut back to dt = 2.10e+06
       max change S.liquid: 0.044 dS.liquid: 0.031 -- tsw35.f#1:1:19
*usnt(17) t 1.01e+07 dt 2.1e+06 ndt 2.1e+06 nr 6 lin 1
       max change S.liquid: 0.044 dS.liquid: 0.031 -- tsw35.f#1:1:24
*usnt(18) t 1.22e+07 dt 2.1e+06 ndt 4.3e+06 nr 7 lin 1
 ==> usnt, max variable change, cut back to dt = 2.94e+06
S.liquid: 0.55 dS.liquid: 0.54 -- tsw35.f#1:1:38
 ==> usnt, hit max. NR iterations, cut back to dt = 1.47e+06
       max change S.liquid: 0.039 dS.liquid: 0.029 -- tsw35.f#1:1:31
*usnt(19) t 1.36e+07 dt 1.5e+06 ndt 1.5e+06 nr 8 lin 1
 ==> usnt, max variable change, cut back to dt = 1.10e+06
S.liquid: 0.4 dS.liquid: 0.39 -- tsw35.f#1:1:45
 ==> usnt, hit max. NR iterations, cut back to dt = 5.51e+05
       max change S.liquid: 0.032 dS.liquid: 0.019 -- tsw35.f#1:1:37
*usnt(20) t 1.42e+07 dt 5.5e+05 ndt 5.5e+05 nr 4 lin 1
 ==> usnt, hit max. NR iterations, cut back to dt = 2.75e+05
       max change S.gas: 0.97 dS.gas: -0.016 -- tsw35.f#1:1:39
*usnt(21) t 1.45e+07 dt 2.8e+05 ndt 2.8e+05 nr 4 lin 1
       max change S.liquid: 0.038 dS.liquid: 0.027 -- tsw35.f#1:1:42
*usnt(22) t 1.47e+07 dt 2.8e+05 ndt 5.7e+05 nr 5 lin 1
       max change S.liquid: 0.046 dS.liquid: 0.036 -- tsw35.f#1:1:46
*usnt(23) t 1.53e+07 dt 5.7e+05 ndt 1.1e+06 nr 8 lin 1
       max change S.liquid: 0.046 dS.liquid: 0.036 -- tsw35.f#1:1:54
*usnt(24) t 1.64e+07 dt 1.1e+06 ndt 2.2e+06 nr 7 lin 1
       max change S.gas: 0.95 dS.gas: -0.037 -- tsw35.f#1:1:60
*usnt(25) t 1.87e+07 dt 2.2e+06 ndt 4.5e+06 nr 8 lin 1
 ==> usnt, hit max. NR iterations, cut back to dt = 2.24e+06
       max change S.liquid: 0.044 dS.liquid: 0.032 -- tsw35.f#1:1:67
*usnt(26) t 2.09e+07 dt 2.2e+06 ndt 2.2e+06 nr 7 lin 1
       max change S.gas: 0.96 dS.gas: -0.029 -- tsw35.f#1:1:73
*usnt(27) t 2.32e+07 dt 2.2e+06 ndt 4.6e+06 nr 5 lin 1
       max change S.liquid: 0.045 dS.liquid: 0.034 -- tsw35.f#1:1:76
```

```
*usnt(28) t 2.77e+07 dt 4.6e+06 ndt 9.2e+06 nr 5 lin 1
       max change S.liquid: 0.049 dS.liquid: 0.026 -- tsw35.f#1:1:79
*usnt(29) t 3.69e+07 dt 9.2e+06 ndt 1.9e+07 nr 5 lin 1
       max change T: 25 dT: -0.14 -- tsw35.m#1:1:2
*usnt(30) t 5.57e+07 dt 1.9e+07 ndt 4.2e+07 nr 2 lin 1
       max change T: 25 dT: -0.29 -- tsw35.m#1:1:2
*usnt(31) t 9.74e+07 dt 4.2e+07 ndt 9.1e+07 nr 2 lin 1
       max change T: 24 dT: -0.57 -- tsw35.m#1:1:2
*usnt(32) t 1.88e+08 dt 9.1e+07 ndt 1.9e+08 nr 2 lin 1
       max change T: 23 dT: -0.97 -- tsw35.m#1:1:2
*usnt(33) t 3.78e+08 dt 1.9e+08 ndt 3.8e+08 nr 2 lin 1
       max change T: 22 dT: -1.4 -- tsw35.m#1:1:2
*usnt(34) t 7.60e+08 dt 3.8e+08 ndt 7.3e+08 nr 2 lin 1
       max change T: 20 dT: -1.5 -- tsw35.m#1:1:2
*usnt(35) t 1.49e+09 dt 7.3e+08 ndt 1.4e+09 nr 2 lin 1
       max change T: 22 dT: -1.4 -- tsw35.m#1:1:3
*usnt(36) t 2.87e+09 dt 1.4e+09 ndt 2.8e+08 nr 2 lin 1
       max change T: 22 dT: -0.26 -- tsw35.m#1:1:3
*usnt(37) t 3.16e+09 dt 2.8e+08 nr 2 lin 1

usnt: total no. of time steps: 37
usnt total no. of N-R iterations: 211
usnt: total no. of func. evaluations: 820
usnt: total no. of matrix iterations: 205

"input" user: 0.01 s. sys: 0 s.; called 1 times
"init." user: 0 s. sys: 0 s.; called 1 times
"char. funs" user: 0.01 s. sys: 0 s.; called 1484 times
"output" user: 0 s. sys: 0 s.; called 38 times
"build eqts" user: 0.22 s. sys: 0 s.; called 205 times
"lin.eqt.soln." user: 0.1 s. sys: 0 s.; called 205 times
"ILU mapping" user: 0 s. sys: 0 s.; called 1 times
total user cpu time: 0.37 s., sys. cpu time: 0 s.
total wall clock time: 0.384 s.
```

4. No error messages were reported.

5. Differences between the "`installation_test_ser.ex`" and "`installation_test_ser_exp.ex`" files were examined by using a "`diff`" command:

```
[carle@aztec3 installation-test]$ diff installation_test_ser.ex
installation_test_ser_exp.ex
5c5
< NUFT version cvs-11-17-04 (LINUX-GCC)
---
> NUFT version cvs-1-13-05 (LINUX-GCC)
100,102c100,102
< $OperatingSystem  Linux nitao1-1.llnl.gov 2.2.5-15smp #1 SMP Mon Apr
19 22:43:28 EDT 1999 i686 unknown
```

```
< $C-Compiler  gcc version 2.95.2 19991024 (release)
< $FortranCompiler  GNU Fortran Front End version 0.5.25 19991024
(release)
---
> $OperatingSystem  Linux thunder2 2.6.9-41.2chaos #1 SMP Mon Jul 17
09:11:20 PDT 2006 ia64 ia64 ia64 GNU/Linux
> $C-Compiler  mpiicpc Version 9.1
> $FortranCompiler  mpiifort Version 9.1
104c104
< $RunDate  Wed Apr 30 15:25:54 2014
---
> $RunDate  Thu Mar 29 15:24:03 2007
```

The differences are a result of different NUFT versions, operating systems, compilers, and run dates. The results of the installation test shown here indicate a successful installation of NUFT on the LLNL AZTEC institutional computer system.

9 Code Review

Under YMP QA, an independent technical review provided oversight of the NUFT code development process (Campbell et al., 1999) using YMP acceptance criteria (CWRMS M&O, 2003) and additional criteria defined by the technical reviewers. All reviewers were scientists and engineers familiar with fluid flow phenomena in accordance with LLNL's YMP procedure YMP-QP 2.10 for qualification of personnel (LLNL, 1992).

10 Configuration Control

Under the YMP QA procedures for Software Configuration Management (CWRMS M&O, 1999) and software management (CRWMS M&O, 2003), LLNL developed a software configuration management system for NUFT (CWRMS M&O, 1998b; Campbell et al., 1999; Levatin and Lewis, 2000; Shaffer, 2000). Configuration control for NUFT v4.0 was updated at LLNL as part of YMP QA assurance (CRWMS M&O, 2007a). LLNL actively supports NUFT software configuration control for NUFT v4.0, including documentation, source code, executables, and operating system components for LLNL institutional and YMP-specific computer systems.

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